

GANs for (fast) simulation



Sofia Vallecorsa for the GeantV team

Outline

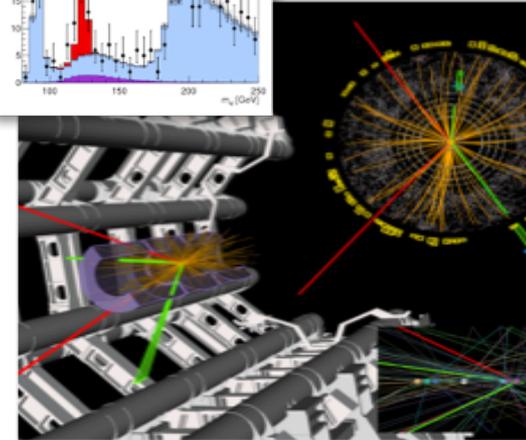
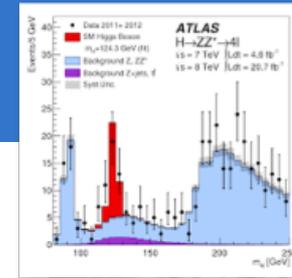
- ▣ Introduction
- ▣ A generic framework for fast simulation
- ▣ GANs for calorimeter showers
- ▣ Summary & Plans

Simulation in HEP

▣ Detailed simulation of subatomic particles is essential for data analysis, detector design

- ▣ Complex physics and geometry modeling
- ▣ Heavy computation requirements, massively CPU-bound

More than 50% of WLCG power is used for simulations



200 Computing centers in 20 countries: > 600k cores

@CERN (20% WLCG): 65k processor cores ; 30PB disk + >35PB tape storage

@HL-LHC needs x100 speed-up in simulation

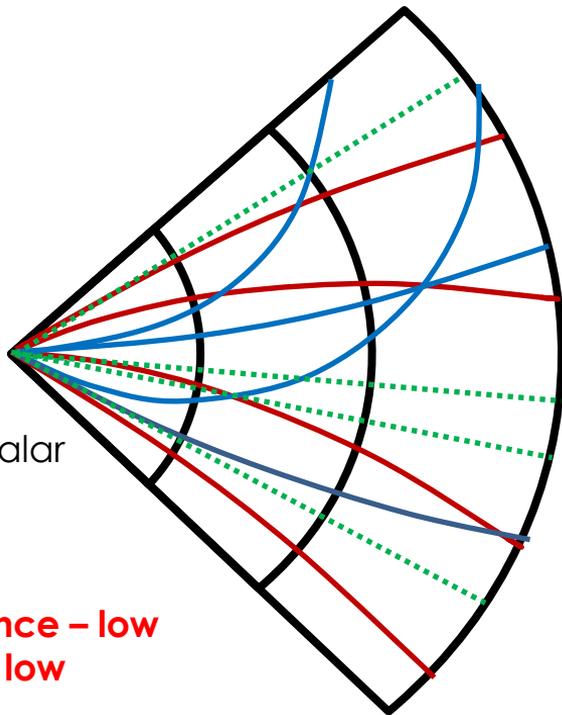
Speeding up simulation

- ▣ State of the art software is Geant4
 - ▣ All particle MonteCarlo transport program
 - ▣ C++ open source simulation toolkit
 - ▣ Capable of handling extremely complex geometries
 - ▣ Large spectrum of applications
 - ▣ Massive and extensive validation
- ▣ Event level multi-threading

GeantV: Adapting simulation to modern hardware

Classical simulation

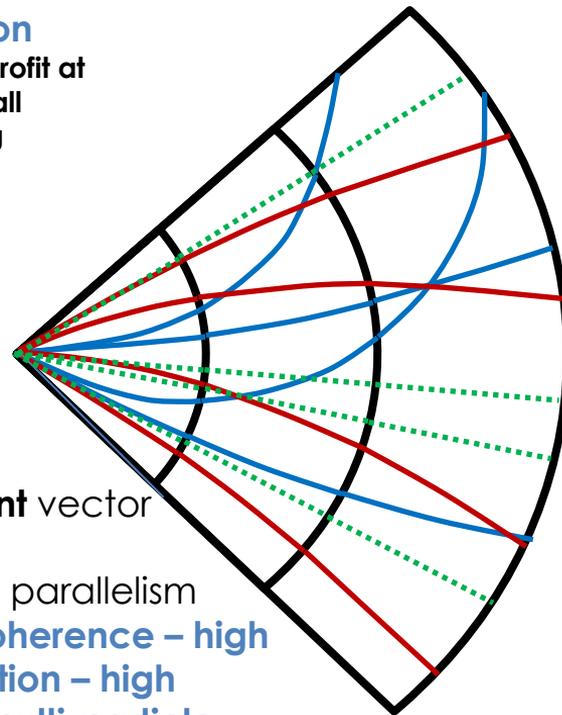
hard to approach the full machine potential



- **Single event** scalar transport
- Embarrassing parallelism
- **Cache coherence – low**
- **Vectorization – low (scalar auto-vectorization)**

GeantV simulation

needs to profit at best from all processing pipelines

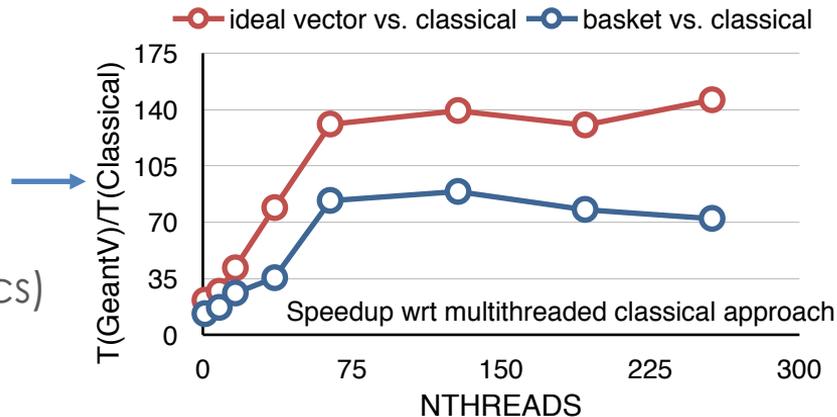
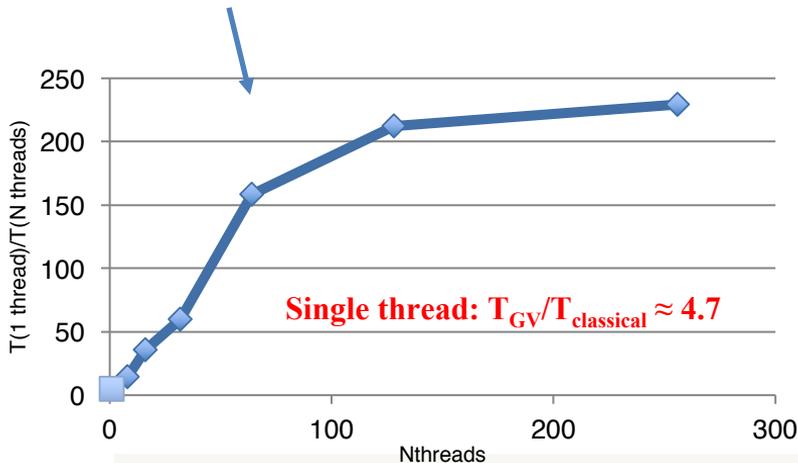


- **Multi-event** vector transport
- Fine grain parallelism
- **Cache coherence – high**
- **Vectorization – high (explicit multi-particle interfaces)**

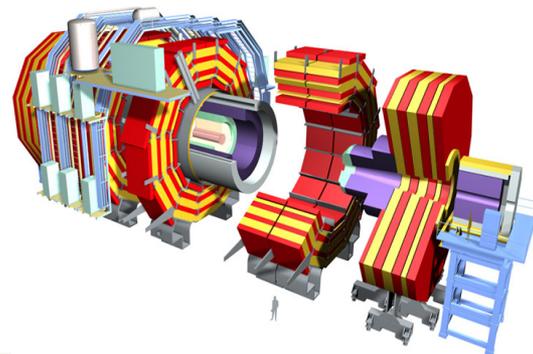


Some benchmarks on multi-cores

- GeantV delivers already a part of the expected performance
- Testing new geometry navigation performance wrt classical (ROOT)
- CMS detector simulation (tabulated physics)



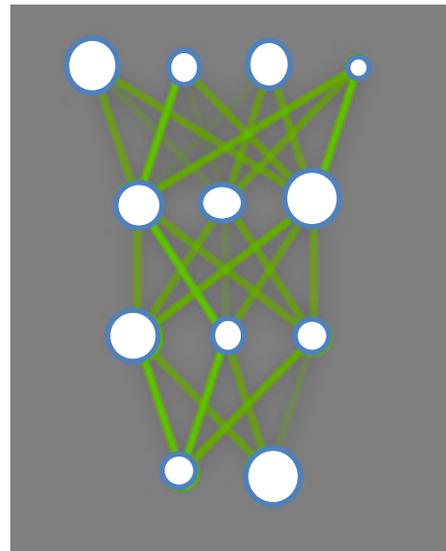
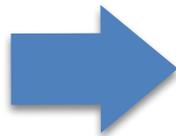
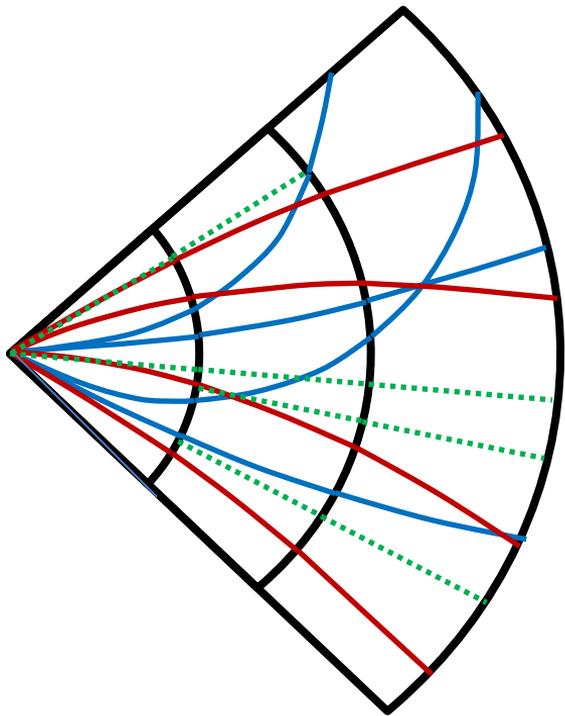
Intel Xeon Phi 7210
@1.30 Hz – 64 cores



Going beyond x10: fast simulation

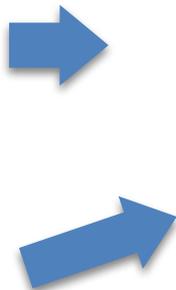
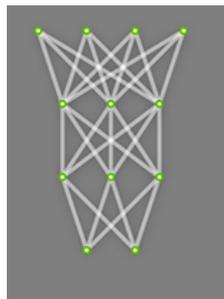
- In the best case scenario GeantV will give $O(10)$ speedup
 - Not enough to cope with HL-LHC expected needs
- Improved, efficient and accurate fast simulation
 - Currently available solutions are detector dependent
- A general fast simulation tool based on Machine Learning techniques
 - Fully configurable interface embedded in GeantV

Going beyond x10: fast simulation

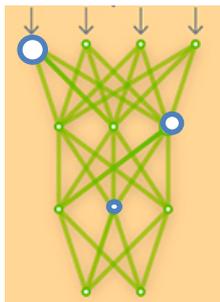


ML engine for fast simulation

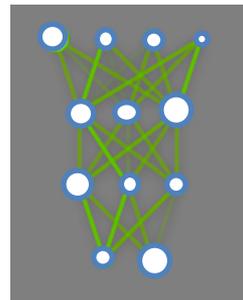
Untrained Model



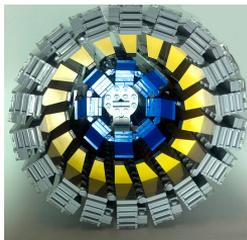
Training



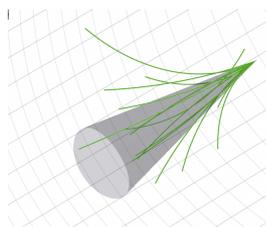
Trained Model



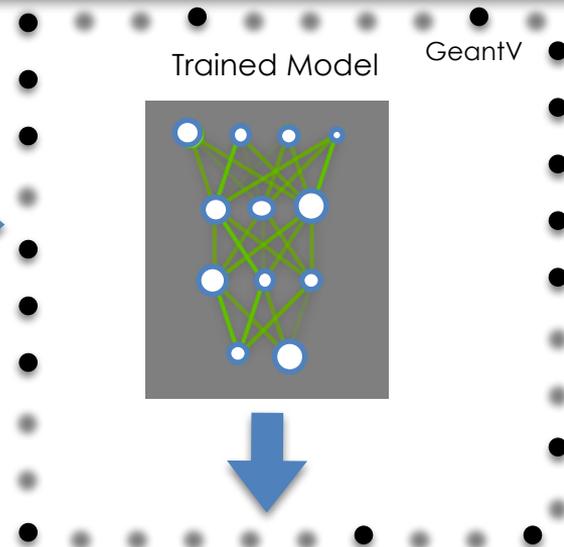
Detector



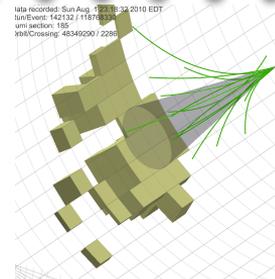
<http://www.physics.umd.edu/rgroups/hep/LegoCMS/>



Physics (e^+ , e^- , γ , π ..)
Kinematics...



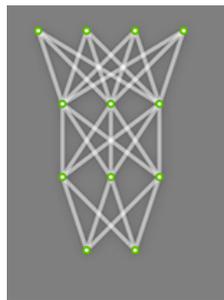
GeantV



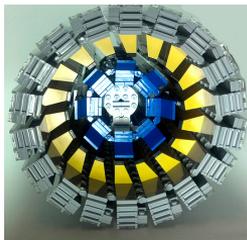
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9th/Crossing: 48349200 / 2289

ML engine for fast simulation

Untrained Model



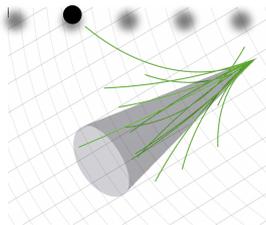
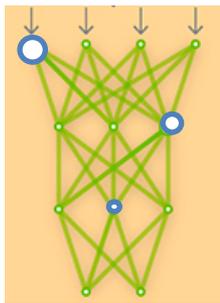
Detector



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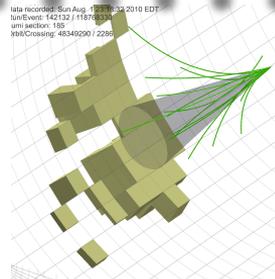
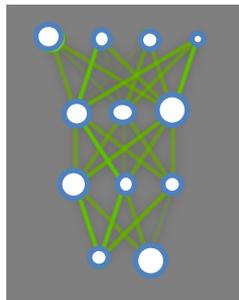
Training



Physics (e^+ , e^- , γ , π ..)
Kinematics...



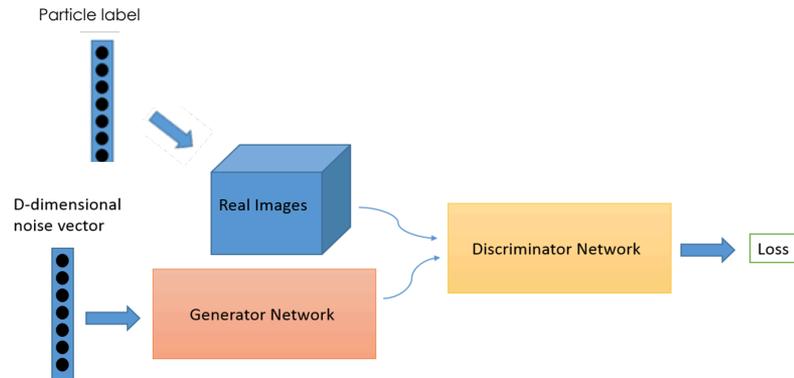
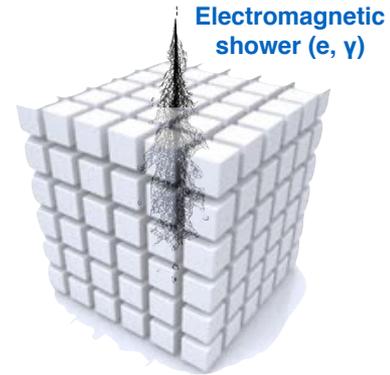
Trained Model



GeantV

Testing GANs for calorimeter images

- ▣ Calorimeters simulation is time consuming
- ▣ Treat energy deposits in cells as 3D image
- ▣ Use LCD ECAL dataset⁽¹⁾

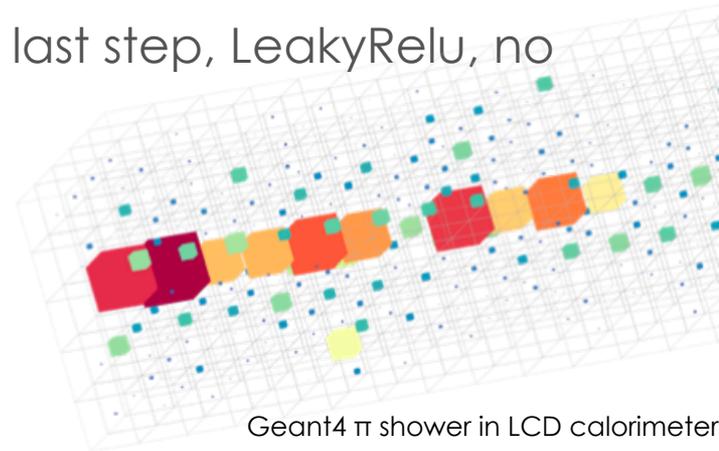
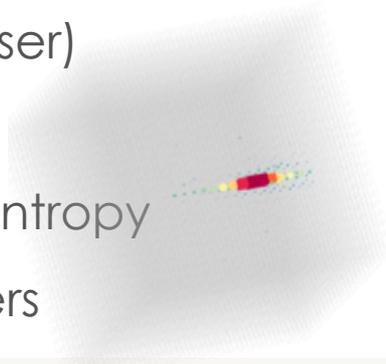


- ▣ Use particle flags to condition the training
- ▣ 3D convolutions using Keras + Tensorflow

(1) See Amir's talk and tutorials

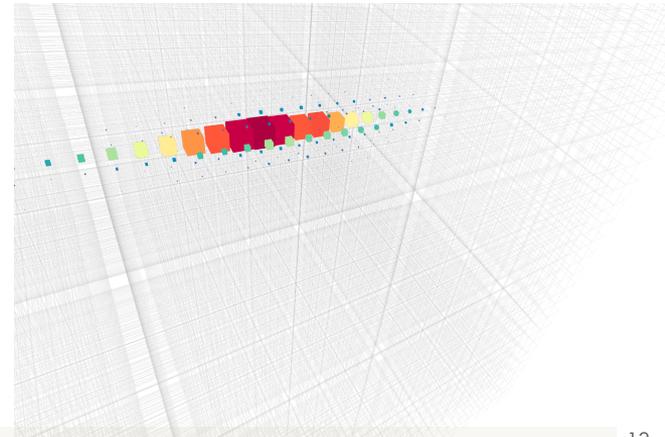
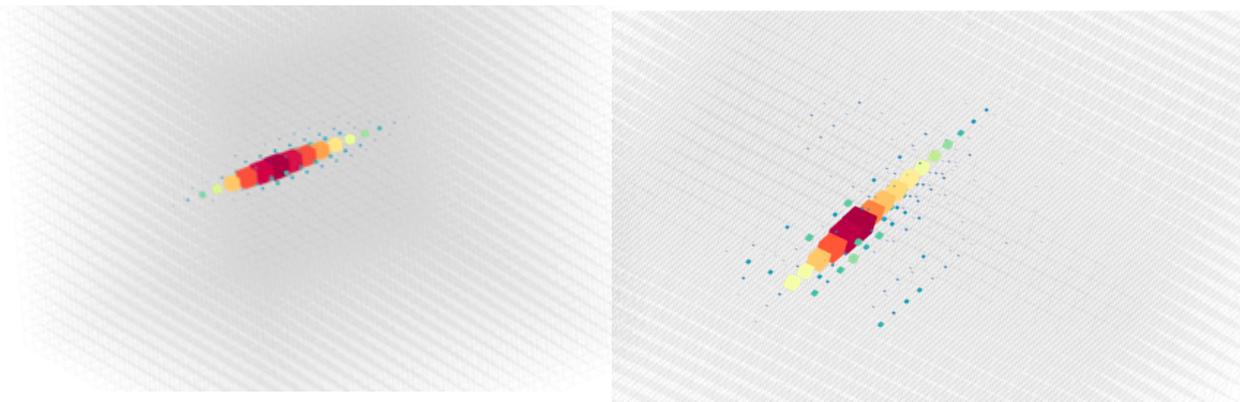
Testing GANs for calorimeter images

- ▣ Similar discriminator and generator models
 - ▣ 3D conv layers with different x,y,z filter sizes
- ▣ Implemented several tips&tricks found in literature
 - ▣ Some helpful (no batch normalisation in the last step, LeakyRelu, no hidden dense layers)
 - ▣ Some not (Adam optimiser)
- ▣ Batch training
 - ▣ Loss is combined cross entropy
 - ▣ Tested different optimisers

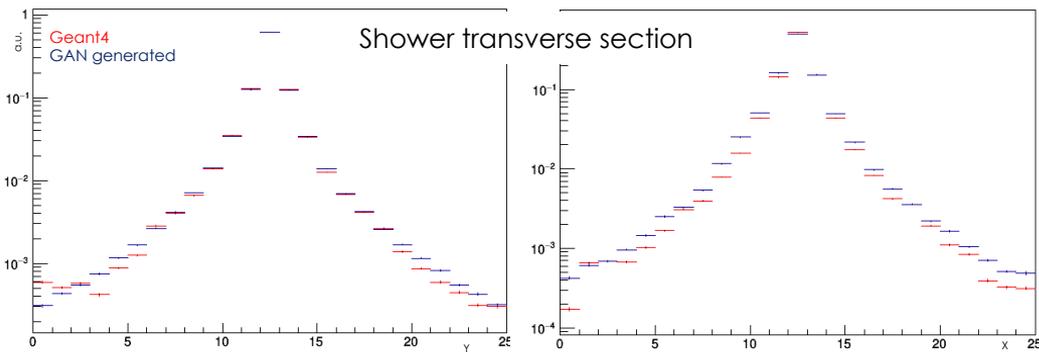


Some images

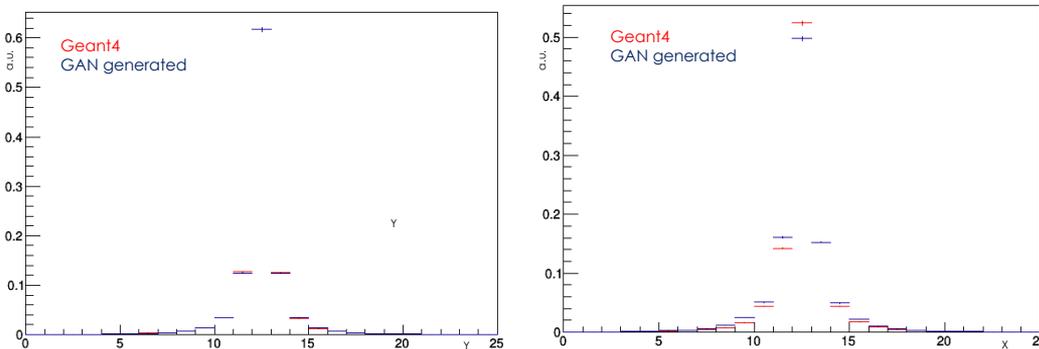
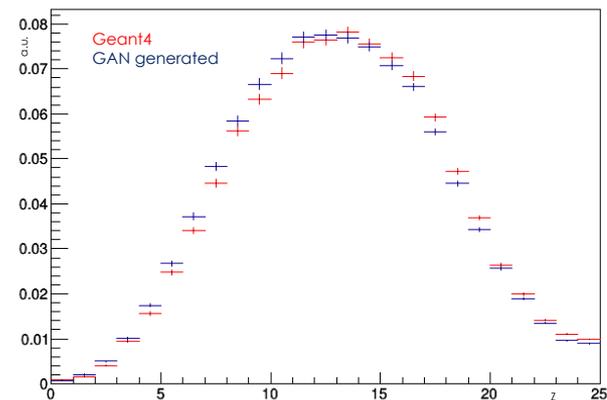
- ▣ Slice energy spectrum
- ▣ Start with photons & electrons



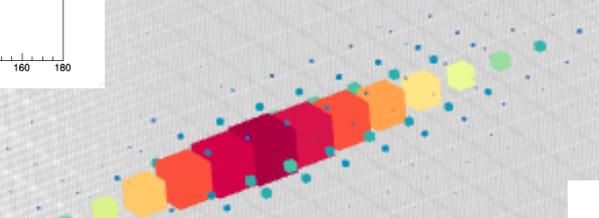
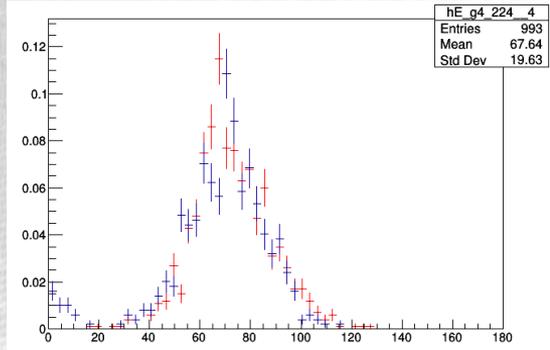
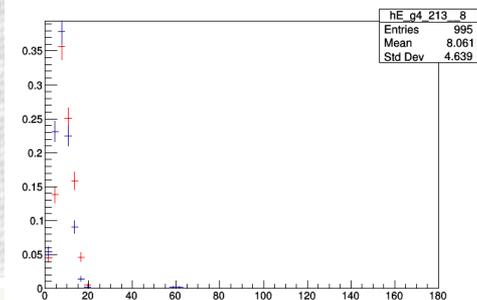
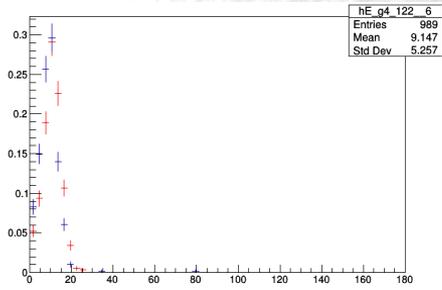
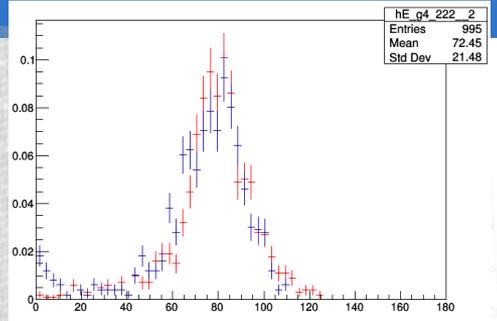
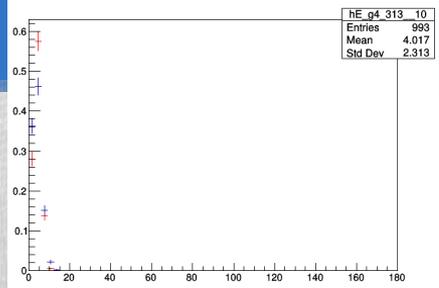
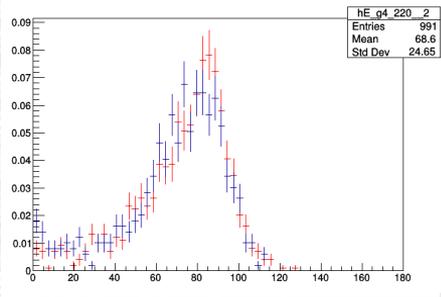
GAN generated electrons



Shower longitudinal section

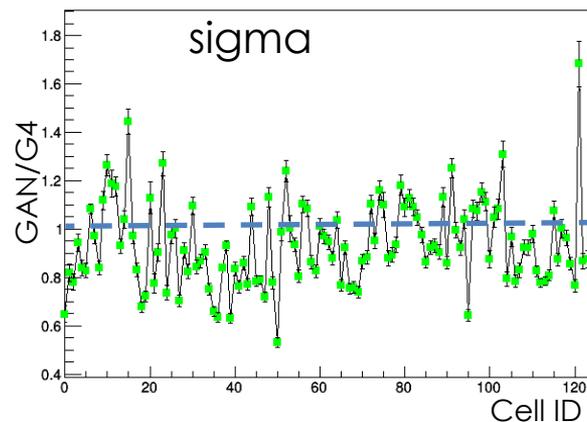
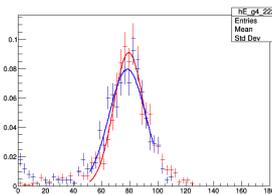
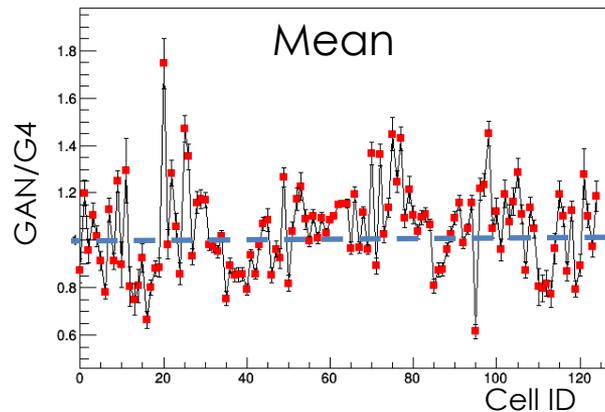


Single cells



Single cells

- Compare energy distribution mean and sigma per cell



- Cell energy sigma is underestimated by GAN
- Set up higher level criteria for image validation (reconstructed variables)

Next steps

- ▣ Detailed study of calorimeter response and comparison to full sim and different fast sim tool
 - ▣ Testing different models to improve physics performance
 - ▣ Include energy info
- ▣ Use information available in the LCD dataset to compare to different techniques (i.e. MO regression)
 - ▣ Test different frameworks
- ▣ Test training on real data

Training time ?

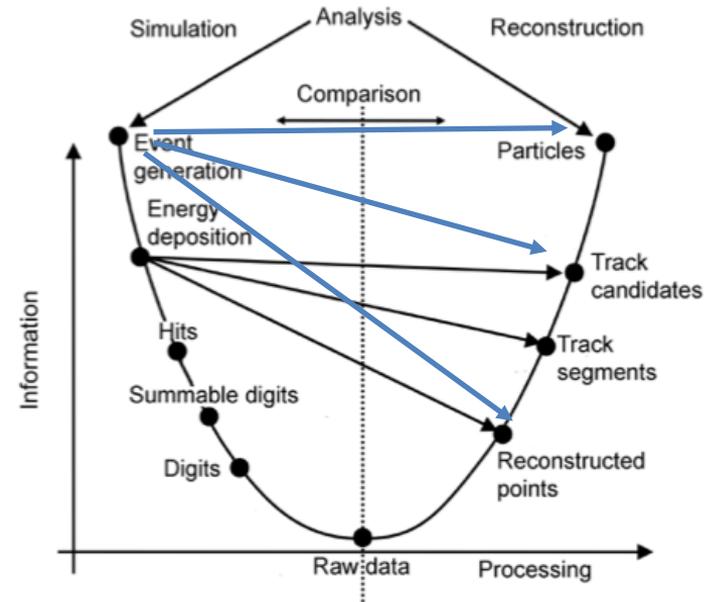
- ▣ Currently adversarial training takes a few hours on NVIDIA GTX1080
 - ▣ Work on the training algorithm
- ▣ Using DL techniques for fast simulation is profitable if training time is not a bottleneck
 - ▣ Depending on the final use case retraining the networks might be necessary
- ▣ Test different hardware & multi-node scaling

Longer term...

- ▣ We want to provide a generic fully configurable tool
 - ▣ Optimal network design depends on the problem to solve
 - ▣ Embedded algorithms for hyper-parameters tuning and meta-optimization
 - ▣ Large hyper-parameter scans
 - ▣ Study parallelization on large clusters
 - ▣ Evaluate existing libraries
 - ▣ Optimize training strategy by reducing communication overhead

Summary

- First images using GANs look very promising
 - Keep working on understanding and improving performance
- Insure computing efficiency and optimal performance on modern hardware
- Initial step of a wider plan to do ML based fast simulation with GeantV
- Even larger speedup gained by replacing digitization and reconstruction steps

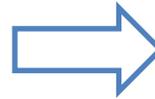
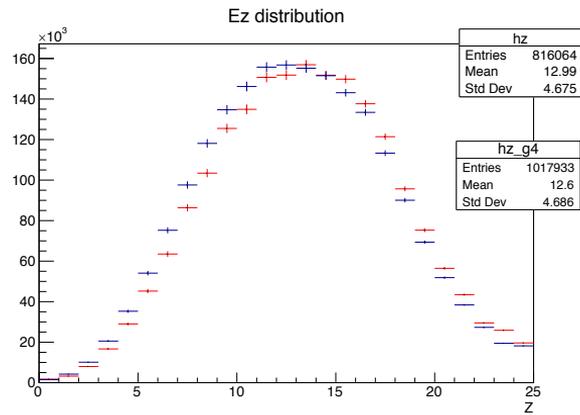




Thank you

..many thanks to M. Pierini and J. Vlimant !

Z filter size = 8



Z filter size = 9

